

Benzonitrile
100-47-0 | DTXSID7021491

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.76e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.62e-01

Confidence level: 7.10e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,4-Benzoquinone

Measured: 4.60e-12

Predicted: 5.97e-12

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1,3,5-Cycloheptatriene

Measured: 9.69e-11

Predicted: 1.00e-10

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(2E)-3-Phenylprop-2-enal

Measured: 4.80e-11

Predicted: 5.31e-11

[Image not found](#)

2-Methyl-p-benzoquinone

Measured: 2.35e-11

Predicted: 2.15e-11